No-go Theorem for One-way Quantum Computing on Naturally Occurring Two-level Systems

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One-way quantum computing achieves the full power of quantum computation by performing single particle measurements on some many-body entangled state, known as the resource state. As single particle measurements are relatively easy to implement, the preparation of the resource state becomes a crucial task. An appealing approach is simply to cool a strongly correlated quantum many-body system to its ground state. In addition to requiring the ground state of the system to be universal for one-way quantum computing, we also want the Hamiltonian to have non-degenerate ground state protected by a fixed energy gap, to involve only two-body interactions, and to be frustration-free so that measurements in the course of the computation leave the remaining particles in the ground space. Recently, significant efforts have been made to the search of resource states that appear naturally as ground states in spin lattice systems. The approach is proved to be successful in spin-$\frac{5}{2}$ and spin-$\frac{3}{2}$ systems. Yet, it remains an open question whether there could be such a natural resource state in a spin-$\frac{1}{2}$, i.e., qubit system. Here, we give a negative answer to this question by proving that it is impossible for a genuinely entangled qubit states to be a non-degenerate ground state of any two-body frustration-free Hamiltonian. What is more, we prove that every spin-$\frac{1}{2}$ frustration-free Hamiltonian with two-body interaction always has a ground state that is a product of single- or two-qubit states, a stronger result that is interesting independent of the context of one-way quantum computing.

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Quantum computers are distinct from classical ones, not only in that they can solve hard problems that are intractable on classical computers, factoring large numbers for example [1], but also in that they can be implemented in architectures such as one-way quantum computing [2–4] that have no evident classical analogues at all. Unlike the quantum circuit model [5–7] which employs entangling gates during the computation, one-way quantum computation requires only single particle measurements on some prepared entangled state, also known as the resource state. This new quantum computation scheme sheds light on the role of entanglement in quantum computation and provides possible advantages in physical implementation of quantum computers. Moreover, from the theoretical computer science perspective, although one-way quantum computations are polynomial time equivalent to the unitary circuit model, they may have advantages over the circuit model in terms of parallelisability [3, 8, 9]. For example, the quantum Fourier transform [10], the key quantum part of Shor's factoring algorithm, is approximately implementable in constant depth in the one-way model [11]. All these nice facts about the one-way computing model make it a worthy topic to pursue both theoretically [12–19] and experimentally [4].

Quantum entanglement is believed to be a necessary ingredient of quantum computation [20, 21]; yet entangling operations used in the unitary circuit model that generate and process quantum entanglement are hard to implement on large scale systems. Entanglement is also essential in one-way quantum computing [22–25]. However, the entanglement used in a one-way quantum computer is cleanly separated in the initial preparation step from the whole computation. Moreover, it usually has a regular structure and is independent of the computation problem and inputs. This allows us to focus on the preparation of some specific entangled resource state.

An appealing idea is to obtain the resource state in some strongly correlated quantum many-body system at low temperature. This approach requires the resource state to be the non-degenerate ground state of some gapped Hamiltonian, which involves only two-body nearest-neighbor interactions. In this way, the resource state can be effectively created via cooling, and the procedure is robust against thermal noises. The Hamiltonian also needs to be frustration free, that is, the ground state minimizes the energy of each local term of the Hamiltonian simultaneously, so that measurements in the course of the computation leave the remaining particles in the ground space.

The canonical resource state for one-way quantum computing, known as the cluster state [2], does not naturally occur as a ground state of a physical system [26]. As a result, there has been significant efforts to identify alternative resource states that appear naturally as ground states in spin lattices [13, 14, 27–29]. In Ref. [28], a natural resource state called triCluster is found in a spin-$\frac{5}{2}$ system. And very re-

cently, a two-body spin-$\frac{3}{2}$ Hamiltonian from a quantum magnet is found, whose unique ground state is also a universal resource state for one-way quantum computing [29]. As two-level systems are more widely available in practice than higher-level systems, it is natural to ask whether there exists a universal resource state in spin-$\frac{1}{2}$ (qubit) system that naturally occurs.

In this letter, however, we show that it is not the case. Namely, a genuinely entangled qubit states cannot be a non-degenerate ground state of any two-body frustration-free Hamiltonian H, as there is always a product of single qubit states in the ground space of H. This indicates that one-way computing with naturally occurring resource states cannot be done with qubits. Therefore, the best one can hope for is to find natural resource state in spin-1 systems, the existence of which remains an open question.

With a similar argument, we show that any two-body frustration-free Hamiltonian has a ground state that is a product of single- or two-qubit states. This leads to deeper understandings of the relationship between frustration in the Hamiltonian and entanglement in the ground state for qubit systems.

It is worth noting that our discussion is also closely related to a problem in quantum computational complexity theory, the quantum analog of 2-Satisfiability (abbreviated as Quantum 2-SAT [30]). We will discussion the relation in detail in the next section.

The frustration-free Hamiltonian.— We start our proof by assuming that there does exist such a naturally occurring state of n qubits, denoted by $|\Psi\rangle$. We also assume for simplicity that the state is genuinely entangled, meaning that it is not a product state with respect to any bi-partition of the n-qubit system.

Given any density matrix ρ, we define its support $\mathrm{supp}(\rho)$ to be the subspace spanned by the eigenvectors of non-zero eigenvalues of ρ. For any two qubits i, j, the two-particle reduced density matrix of these two qubits of state $|\Psi\rangle$ is denoted as ρ_{ij}.

The state $|\Psi\rangle$ gives rise to a two-body frustration-free Hamiltonian H_Ψ that has $|\Psi\rangle$ in its ground space, and at the same time, has the smallest possible ground space in a sense formalized below. In fact, the Hamiltonian can be chosen, without loss of generality, to be the sum of projections Π_{ij} onto the orthogonal space of the $\mathrm{supp}(\rho_{ij})$, that is,

$$H_\Psi = \sum_{ij} \Pi_{ij}. \tag{1}$$

As H_Ψ is constructed from state $|\Psi\rangle$, we call it the two-body frustration-free Hamiltonian of $|\Psi\rangle$

Clearly H_Ψ is two-body and frustration-free, and $|\Psi\rangle$ is a ground state of H_Ψ with energy 0. Note that the ground space of H_Ψ is given by

$$\mathcal{S}(|\Psi\rangle) = \bigcap_{ij} \mathrm{supp}(\rho_{ij} \otimes I_{\bar{i}\bar{j}}), \tag{2}$$

where $I_{\bar{i}\bar{j}}$ is the identity operator on qubits other than i, j.

Generally, a frustration-free Hamiltonian H needs not to be a summation of projections. However, we can always find one whose local terms are indeed projections and has the same ground space as H. Therefore, we only consider frustration-free Hamiltonian that are summation of projections in this paper. It is not hard to see that any two-body frustration-free Hamiltonian H' that has $|\Psi\rangle$ as a ground state also contains $\mathcal{S}(|\Psi\rangle)$ in its ground space. In other words H_Ψ has the smallest possible ground space among all frustration-free Hamiltonians having $|\Psi\rangle$ as a ground state.

There is a natural correspondence between a two-body frustration-free Hamiltonian H and the Quantum 2-SAT problem. Classically, a 2-SAT problem asks whether a logical expression in the conjunctive normal form with two variables per clause, e.g. $(x_0 \vee x_1) \wedge (\neg x_1 \vee x_2) \wedge (x_2 \vee \neg x_0)$, is satisfiable or not, where x_i are Boolean variables and $\wedge, \vee, \neg$ are logical AND, OR, NOT operations. There is a well-known polynomial time classical algorithm that solves 2-SAT while the related 3-SAT problem is believed to be much harder (NP-Complete [31]). In Ref. [30], it was proved that the quantum analog of the 2-SAT problem, which asks whether a set of projections on two-qubit subsystems has a simultaneous ground state, is also efficiently solvable on a classical computer. It was also shown there that Quantum 4-SAT is one of the hardest problems in QMA_1 (a quantum analog of NP [31]), meaning that it is probably hard even for quantum computers. The relation between a frustration-free Hamiltonian and its corresponding quantum SAT problem is evident. The Hamiltonian H is indeed frustration-free, thereby having 0 ground energy, if and only if the quantum SAT problem defined by the set of projections in the Hamiltonian H is satisfiable. In the case of two-body Hamiltonian H_Ψ, the corresponding Quantum 2-SAT problem is defined by Π_{ij}'s. If for each term Π_{ij}, the rank of it is either 0 or 1, the corresponding Quantum 2-SAT problem is called homogeneous [30], a concept that will be used in the following.

Now we go back to the Hamiltonian problem and show that $|\Psi\rangle$ cannot be a unique ground state of any two-body frustration-free Hamiltonian by proving the following theorem.

Theorem 1. *Given an n-qubit state $|\Psi\rangle$ that is genuinely entangled and any two-body frustration-free Hamiltonian H having $|\Psi\rangle$ as its ground state. There always exists a product state of single qubits also in the ground space of H for $n \geq 3$.*

As H_Ψ has the smallest ground space, we only need to prove the theorem for H_Ψ instead of the general H. Also, it is equivalent to prove that $\mathcal{S}(|\Psi\rangle)$ is of dimension at least 2 and contains a product state of single qubits.

Proof of the theorem.— We prove this theorem by induction. Before doing so, we examine the following fact. Let $|\Psi\rangle$ and $|\Phi\rangle$ be two n-qubit states that can be transformed into each other by invertible local operations. That is, there are 2×2 non-singular linear operators $L_1, \cdots, L_n$, such that $|\Psi\rangle = \mathcal{L}|\Phi\rangle$, where $\mathcal{L} = L_1 \otimes \cdots \otimes L_n$. This is equivalently to saying that $|\Psi\rangle$ and $|\Phi\rangle$ can be transformed to each

other via stochastic local operation and classical communication (SLOCC) [32, 33]. Noticing the fact [34] that $|\Psi\rangle$ is a ground state of H if and only if $|\Phi\rangle$ is a ground state of

$$H' = \sum_{ij} (L_i \otimes L_j)^\dagger \Pi_{ij} (L_i \otimes L_j), \tag{3}$$

and the trivial fact that $\mathcal{L}$ maps product states to product states, we only need to discuss states that are representatives of equivalent classes induced by such local transforms $\mathcal{L}$. Equivalently, it suffices to consider SLOCC equivalent classes.

For three-qubit genuinely entangled states, there are only two different SLOCC equivalent classes [33], represented by the $|W\rangle$ and $|GHZ\rangle$ respectively where $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$, and $|GHZ\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$. For the $|W\rangle$ state, one has

$$\mathcal{S}(|W\rangle) = \mathrm{span}\{|W\rangle, |000\rangle\}, \tag{4}$$

therefore the product state $|000\rangle$ is in the ground space. While for $|GHZ\rangle$,

$$\mathcal{S}(|GHZ\rangle) = \mathrm{span}\{|000\rangle, |111\rangle\}, \tag{5}$$

both product states $|000\rangle$ and $|111\rangle$ are in the ground space. This then proves the theorem for the three-qubit case.

Now we proceed to the four-qubit case. Note that $|\Psi\rangle$ is genuinely entangled, all ρ_{ij} must be of rank at least 2, i.e. the dimension of the $\mathrm{supp}(\rho_{ij})$ is at least 2 and the rank of Π_{ij} is at most 2. We will discuss two cases here.

Case 1. If for some pair of qubits, say $(3, 4)$, the rank of their reduced density matrix ρ_{34} is 2, then the pair of qubits $3, 4$ can be encoded as a single qubit. Therefore, we can reduce our problem to a similar one of smaller system size.

To be more precise, suppose ρ_{34} is supported on two orthogonal states $|\psi_0\rangle_{34}$ and $|\psi_1\rangle_{34}$. Define an isometry

$$V : |0\rangle_{3'} \to |\psi_0\rangle_{34}, |1\rangle_{3'} \to |\psi_1\rangle_{34}, \tag{6}$$

which maps a single qubit to two qubits. That is, we have used qubit $3'$ to encode the two qubits $3, 4$. Define $|\Phi\rangle = V^\dagger|\Psi\rangle$, so $|\Psi\rangle$ is a ground state of H if and only if $|\Phi\rangle$ is a ground state of $H' = V^\dagger H V$. One can easily verify that H' is still a two-body frustration-free Hamiltonian and $|\Phi\rangle$ is a genuinely entangled state of 3 qubits. This reduces to a case already proved and there is product state $|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_{3'}\rangle$ which is also a ground state of H'.

Let $|\beta_{34}\rangle$ be $V|\alpha_{3'}\rangle$, a two-qubit state of qubits $3, 4$. If it is a product state, then we are done. If it is entangled, as ρ_{34} is supported on a 2-dimensional space, there always exists a product state $|\beta_3\rangle \otimes |\beta_4\rangle \in \mathrm{supp}(\rho_{34})$ [35]. Consider now the bi-partition between qubits $1, 2$ and qubits $3, 4$. As $|\beta_{34}\rangle$ is entangled, any projection term that concerns two qubits from different partitions will have trivial constraints on qubits 3 and 4. Therefore, the product state $|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\beta_3\rangle \otimes |\beta_4\rangle$ is also a ground state of H.

Case 2. If all of the $\mathrm{supp}(\rho_{ij})$ are of rank 3 or 4, we employ the homogeneous 2-SAT and completion techniques in Ref. [30] to finish the proof. The completion procedure adds possibly new projection terms to the frustration-free Hamiltonian without changing the ground space. For any three qubits, say $1, 2, 3$, the procedure takes two rank-1 Hamiltonian terms say Π_{12} and Π_{23}, and generates a possibly new constraint Ω_{13}. See Fig. 1 for an illustration. We briefly review the specific rule for obtaining Ω_{13} from Π_{12} and Π_{23}; and refer the interested readers to Ref. [30] for the proof and details. Let $\Pi_{12} = |\phi\rangle\langle\phi|$, $\Pi_{23} = |\theta\rangle\langle\theta|$, and $\Omega_{13} = |\omega\rangle\langle\omega|$, where $|\phi\rangle, |\theta\rangle, |\omega\rangle$ are two-qubit pure states. Denote, for example, $\phi_{\alpha,\beta}$ as the amplitude $\langle\alpha, \beta|\phi\rangle$. Then relation is given by $\omega_{\alpha,\gamma} = \phi_{\alpha,\beta}\epsilon_{\beta,\delta}\theta_{\delta,\gamma}$, where $\epsilon = |0\rangle\langle 1| - |1\rangle\langle 0|$ and the summation of repeated indices is implicit [30].

The key point here is that the construction of H_Ψ guarantees that no new constraint could ever been added during the completion procedure. Therefore, H_Ψ corresponds to a Quantum 2-SAT that satisfies all the conditions (homogeneous and completed) in Lemma 2 of Ref. [30] and it follows that there is a product of single-qubit states in the ground space of H_Ψ.

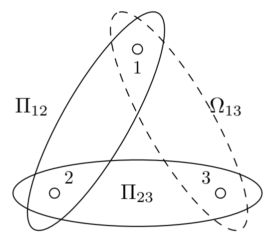

FIG. 1: An illustration of completion procedure

This proves the theorem for the four-qubit case and the general n-qubit case can be proved by the same induction.

Entanglement versus frustration for qubit system.— Our main result is a no-go theorem for one-way quantum computing, which says that in order to do one-way quantum computing with a natural ground state, one has to go to higher dimensional particle systems other than two-level systems. Interestingly, a similar argument also gives a better understanding for the relationship of entanglement and frustration for qubit systems. We can modify our method to show the following result.

Theorem 2. *For any two-body frustration-free Hamiltonian H of a qubit system, there always exists a ground state, which is a product of single- or two-qubit states.*

To see this, first note that if any local term Π_{ab} in H is of rank 3, then the corresponding ground state can only be of the form $(I - \Pi_{ab}) \otimes |\Psi'\rangle\langle\Psi'|$, where $(I - \Pi_{ab})$ is of rank 1 and $|\Psi'\rangle$ is a state of remaining qubits. Secondly, as the Hamiltonian is now of a more arbitrary form, we may not automatically have the completion property as in H_Ψ. Yet, it is easy to overcome this problem by the use of completion procedure as in Ref. [30] and we omit the details for simplicity.

This theorem indicates that frustration is a necessary condition for genuine many-body ground state entanglement in a natural qubit system with non-degenerate ground state.

In the language of Quantum 2-SAT, the above theorem states that if a Quantum 2-SAT is satisfiable, there will be a ground state that is product of single- or two-qubit states. This is a much simpler form than the recursive construction in Ref. [30].

If we further require some symmetry of the Hamiltonian, say, certain kind of translational invariance, there could be only two phases for a non-degenerate frustration-free system with qubits at zero temperature: one is a product state phase, and the other is a dimer phase [36]. This relationship of entanglement and frustration is not true in a spin-1 (qutrit) system. For instance, the famous Affleck-Kennedy-Lieb-Tasaki (AKLT) state [37] is a non-degenerate ground state of a two-body frustration-free Hamiltonian on a chain. Interestingly, the AKLT state and some of its variants on a chain are indeed powerful enough to process single qubit information in the one-way quantum computing model [13, 19, 27, 38].

Summary and Discussion.— We have shown that it is impossible for a genuinely entangled qubit state to be a unique ground state of any two-body frustration-free Hamiltonian H, because there is always a product state of single qubits also in the ground space of H. This indicates that one-way computing cannot be done on naturally occurring qubit systems. Furthermore, we use similar technique to prove that every spin-$\frac{1}{2}$ frustration-free Hamiltonian with two-body interaction always has a ground state that is a product of single- or two-qubit states. These results are strong in the sense that they are independent of the lattice structure, and therefore valid for any lattice geometry with natural nearest-neighbour interactions in the Hamiltonian.

A direct consequence also follows for condensed matter theory. Namely, without degeneracy, there is no genuine many-body entanglement in a ground state of a spin-$\frac{1}{2}$ frustration-free Hamiltonian with two-body interaction. This is not the case for frustration-free higher spin systems or spin-$\frac{1}{2}$ systems with more than two-body interactions. These observations are also closely related to the study of quantum computational complexity theory, which shows that Quantum 2-SAT is easy, but Quantum 2-SAT with large enough local dimensions or Quantum 3-SAT might be much more difficult [30, 39]. Our result also simplifies the structure of the solution space of Quantum 2-SAT given in Ref. [30]. However, a full characterization of the solution-space structure needs further investigation. We hope that our result helps in further investigations of local Hamiltonian problems and in linking the fields of condensed matter, quantum information and computer science.

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